Efficient Implementation for Unitary Coupled Cluster State Preparation for Near-Term Quantum Computers

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Unitary coupled cluster theory (UCC) is a common wave function ansatz for quantum simulation of molecular electronic structure using the variational quantum eigenvalue solver (VQE). Even for small molecules using a double-ζ basis, the number of variational parameters required to minimize the electronic energy (i.e., optimize the circuit) is large and beyond the reach of current quantum computers. For example, a circuit simulating C_2 using the UCCSD ansatz and the cc-pVDZ basis set with frozen-core will require over 10,000 variational parameters and a Hilbert space of over 10^8 determinants. To make progress on simulating such molecular systems on near-term quantum computers, we explore how much of the optimization can be approximately prepared with classical simulation while reducing the number of optimization steps performed on a quantum device. Recently, Chen, Cheng, and Freericks [*J. Chem. Theory Comput.* **2021**, *17*, 841-847] presented an algorithm for the factorized form of the UCC ansatz that allows for efficient UCC optimizations on classical hardware. We flip the algorithm around and use it to prepare approximate quantum circuits for systems that require a large number of qubits to represent. We will present results from our implementation and discuss strategies for incorporating this implementation for algorithms involving near-term quantum computers.